Surrogate model approach for improving the performance of reactive transport simulations

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Aim and Motivation

We **aim to build a system for enabling high-speed reactive transport simulations** spanning millions of elements. Such simulations involve at least two coupled simulation models:

- a hydrodynamics simulator (fast, solved globally)
- geochemical simulation model (slow, solved element-wise)

Problem

Slowness of geochemical simulators makes reactive transport simulations spanning millions of spatial elements practically impossible.

Approach

We propose to **replace** the coupled **geochemical simulation model with a surrogate model,** trained on the input-output data of the simulation model.

Challenge

The **surrogate model** needs to **use the results of its predictions**, modified by transport model, **as inputs at each subsequent time-step** (Fig. 1).

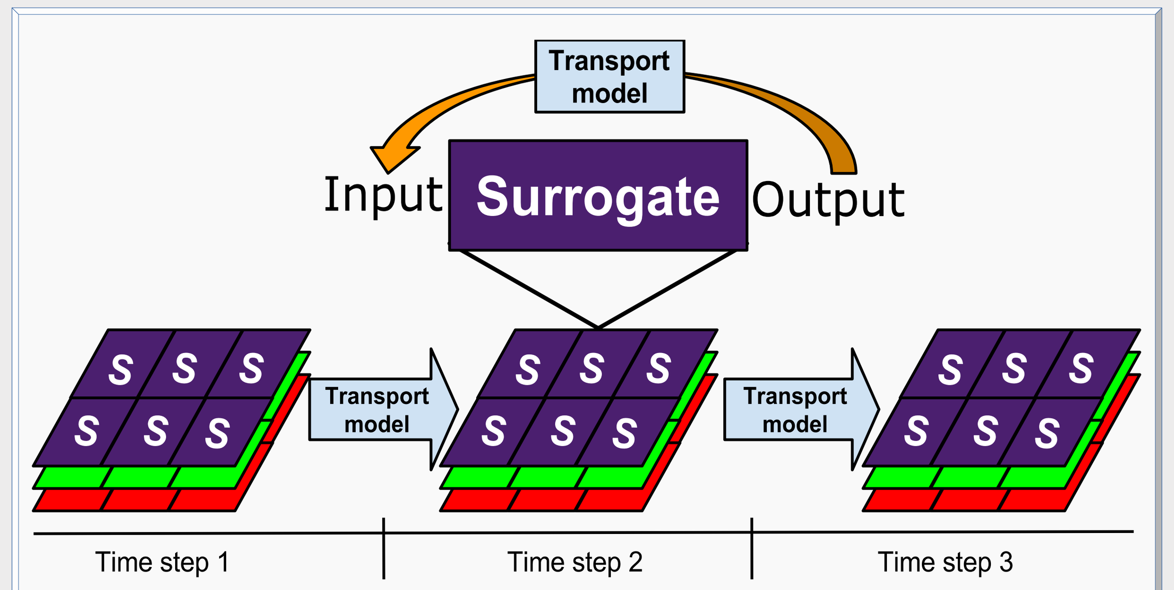

Fig. 1. Using the surrogate model in place of geochemical simulator for reactive transport simulation

Methods

We developed and tested a proof-of-concept surrogate model approach on a well-known 1D reactive transport benchmark problem (Kolditz et al., 2012).

We did this by training 224 statistical model and preprocessor combinations for use as surrogate models. We then compared their accuracy using global error measures. The best performing surrogate model candidates were then used to replace the simulation model in the reactive transport simulation.

Results

Several method and preprocessor combinations perform well according to global error measure (Fig.2), but we find BRNN (shown in Fig. 3) and QRNN to be better suited for replacing the simulator, because:

- PPR produces inconsistent output
- QRF is slower in prediction than the simulation model itself
- MARS shows promising results, but is worse than BRNN and QRNN
- Linear models are not better than MARS

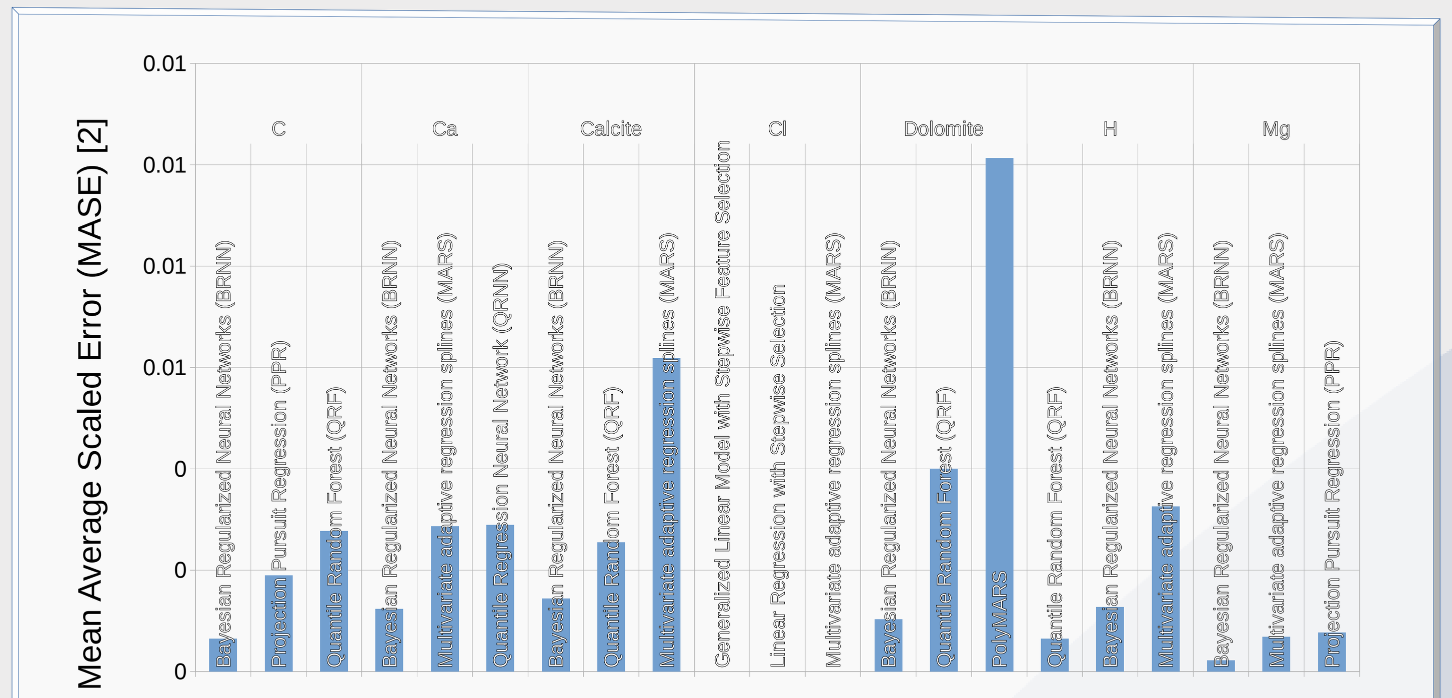

Fig. 2. Top 3 surrogate methods for each simulator output

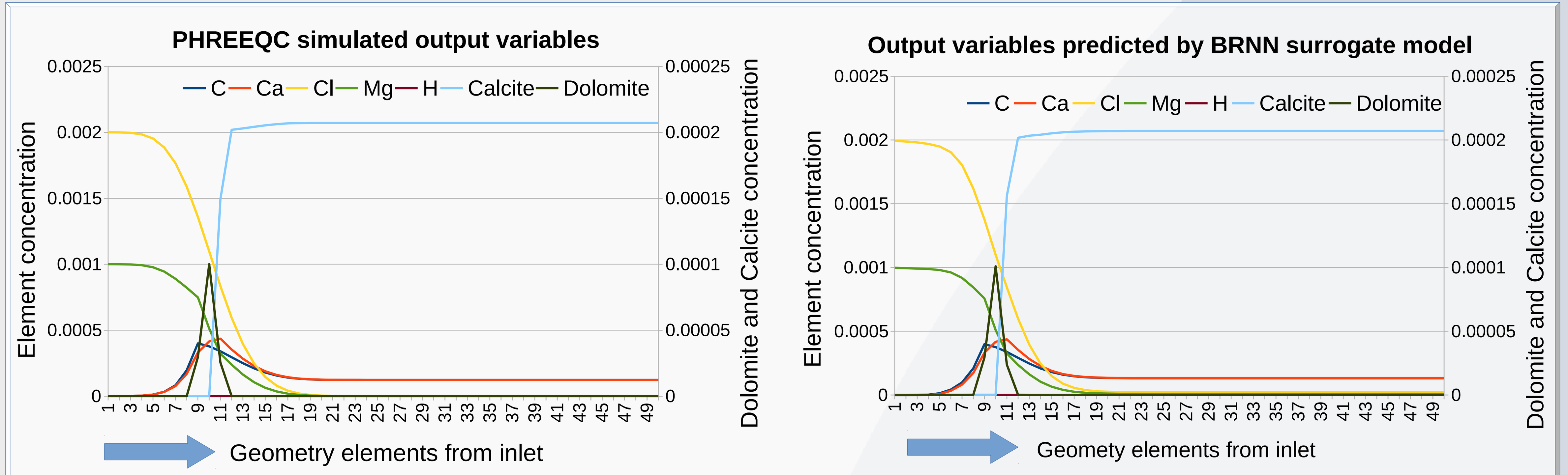

Fig. 3. Simulator vs Surrogate performing reactive transport (timestep 100 of 197)

Is using the surrogate model "worth it"?

Depending on the surrogate model replacing the geochemical simulation model for this scenario, the speed can improve ~50-140 times (Fig. 4).

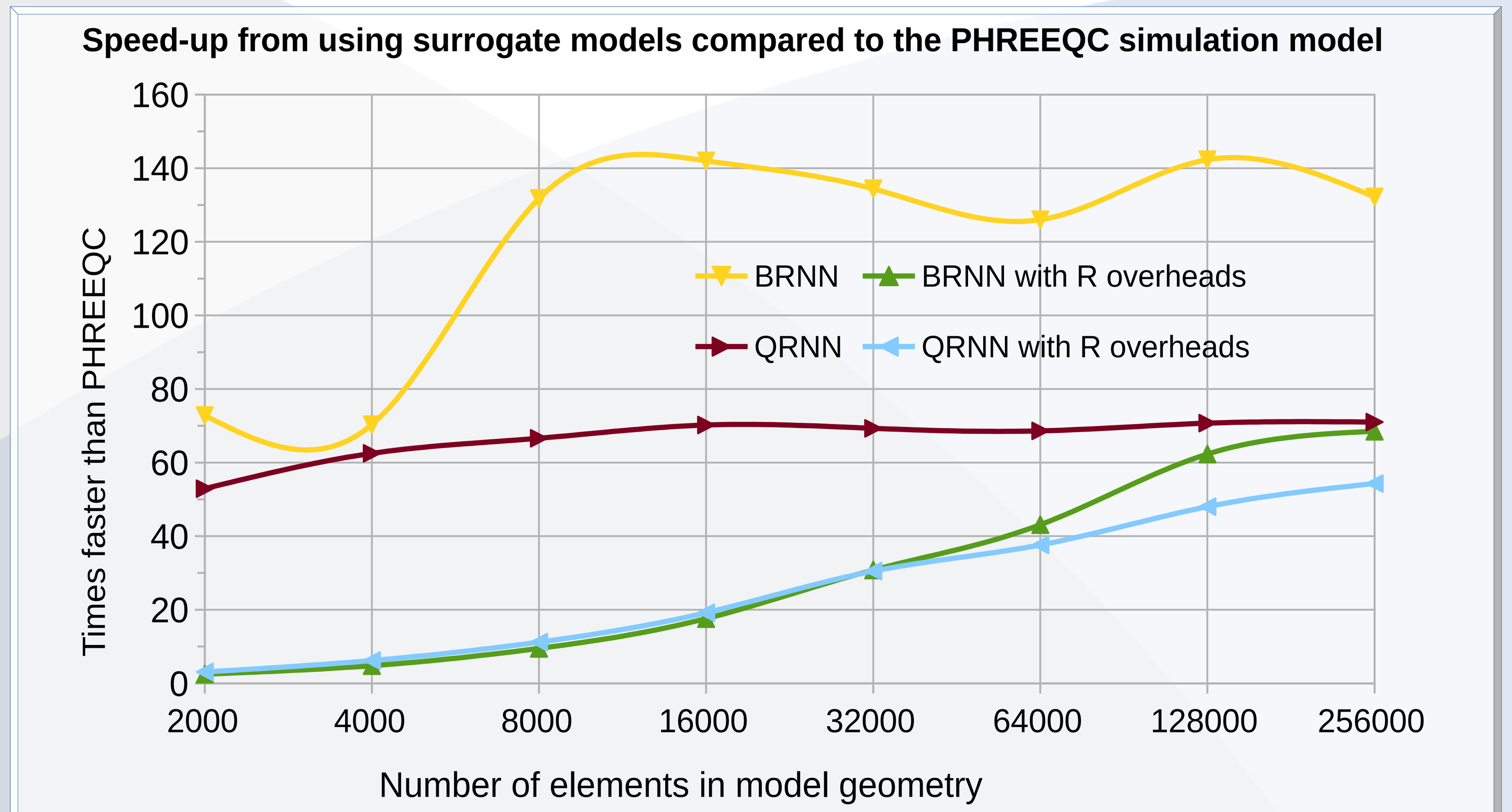

Fig. 4. Surrogate speed by number of geometry elements

Conclusions

- We demonstrate a proof-of-concept for replacing the geochemical simulation model with a surrogate model for use in reactive transport simulation.
- To the best of our knowledge this is the first time this is demonstrated in context of the main challenge (Fig.1).
- The benefits of using the surrogate model increase with the number of geometry elements (Fig.4).

Future work

We aim to make reactive transport simulations possible for model geometries spanning millions of elements. To achieve this we plan to:

- Create a systematic interactive visualization approach to support this currently complex work-flow for different scenarios.
- Use enhanced sampling strategies and support interactive selection and tuning of the better performing statistical models.

References

1. Kolditz, O., Görke, U.J., Shao, H. and Wang, W., 2012. Thermo-hydro-mechanical-chemical processes in porous media: benchmarks and examples (Vol. 86). Springer Science & Business Media.
2. Hyndman, R.J. and Koehler, A.B., 2006. Another look at measures of forecast accuracy. International journal of forecasting, 22(4), pp.679-688.